

Isospin Splittings in the Light Baryon Octet from Lattice QCD+QED at the Physical Mass Point

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Electromagnetic effects and the up-down quark mass difference have small but highly important effects on octet baryon masses. A prominent example is the stability of the hydrogen atom against beta decay. Here we report on a calculation¹ that includes these effects by adding them to valence quarks in an $N_f=2+1$ lattice Quantum Chromodynamics calculation based on ensembles with 5 lattice spacings down to 0.054 fm, lattice sizes up to 6 fm, and average up-down quark masses all the way down to their physical value. This large parameter space allows us to gain control over all systematic errors, with the exception of the one associated with neglecting electromagnetism in the sea. We compute the octet baryon isomultiplet mass splittings, as well as the individual contributions from electromagnetism and the up-down quark mass difference. Our results for the total splittings are in good agreement with experiment.

1 Introduction

All observed particle physics phenomena are accurately described by an $SU(2)_L \times U(1)_Y \times SU(3)_c$ relativistic quantum gauge theory known as the Standard Model. In this theory, the $SU(2)_L \times U(1)_Y$ component explains the weak and electromagnetic interactions, while the $SU(3)_c$ component, known as Quantum Chromodynamics (QCD), describes the strong interaction between quarks and gluons. For light or heavy-light hadron processes, the Standard Model reduces to an $SU(3)_c \times U(1)_{em}$ gauge theory, where the $U(1)_{em}$ stands for Quantum Electrodynamics (QED).

Simulations of QCD use the lattice regulated theory, called lattice QCD. Present-day, state-of-the-art lattice QCD computations are performed in the isospin limit, in which it is assumed that the u and d quarks are mass degenerate (i.e. $m_u = m_d = m_{ud} \equiv (m_u + m_d)/2$) and in which electromagnetism is neglected. This framework is known as $N_f = 2$ or $N_f = 2 + 1$ (if strange sea quarks are included) lattice QCD. In this framework, we have recently obtained important results amongst which are those for the light hadron spectrum², for the average up-down and strange quark masses^{3,4}, for the $SU(3)$ -flavour breaking effects in the ratio of leptonic decay constants f_K/f_π ⁵. These results were obtained with fully controlled, combined statistical and systematic errors on the few percent level.

Given this important progress and the fact that we are now reaching percent level accuracies in our QCD computations, it is becoming critical to include QED and quark-mass isospin breaking effects, the last ingredients required to claim to have a full Standard Model description of quark processes at low energies.

While QED and isospin breaking effects are small for most hadronic quantities, their consequences far surpass their numerical size. For instance, they are strongly believed to be responsible for the fact that neutrons are heavier than protons, thereby ensuring the existence of stable atoms and, more generally, of the large majority of visible matter in the universe. Moreover, they are required to determine the individual up and down quark masses *ab initio*. This is important because a vanishing up quark mass, $m_u = 0$, would provide a very elegant solution to the strong CP problem. Though this possibility is very unlikely given present knowledge⁶, it will only be ruled out for certain when isospin breaking corrections are fully calculated. The determination of the individual u and d quark masses is intimately related to the corrections to Dashen's theorem⁷, which have been the object of heated debates ever since its formulation. In addition, thanks to the progress made recently in lattice simulations, a number of very important theoretical predictions for particle physics have errors in the range of a few percent. With isospin breaking corrections parametrically on the order of about 1%, it is clear that for further progress to be made, they will have to be included.

Here, we report on a calculation¹ aiming to compute the aforementioned neutron-proton mass difference as well as the remaining octet baryon isomultiplet mass splittings. The isospin quark mass splittings are included in the partially quenched approximation and electromagnetic effects in quenched QED. Our results for the individual quark masses and the implications on Dashen's theorem will be discussed in an upcoming publication⁸.

2 Simulation

Our simulation setup is the following^{1,9–11}: in order to study QED and isospin-breaking ($m_u - m_d = \delta m < 0$) effects on hadron properties, we simulate three flavours of quarks (at physical mass parameter values) and QED in the valence sector, using our 47, 2010 ensembles^{3,4} with 5 lattice spacings down to 0.054 fm, lattice sizes up to 6 fm and average up-down quark masses all the way down to their physical value. In this way, we take the dominant effects induced by QED and isospin breaking into account: since mass and e.m. isospin symmetry breaking corrections are small and of comparable size, it is legitimate to expand the standard model in powers of δm and α , assuming $O(\delta m) \sim O(\alpha)$ (and $O(\delta m^n)$, δm to be normalised by a typical QCD mass scale). Given the magnitude of the expansion parameters, this expansion is expected to converge very rapidly, with each subsequent order contributing $\sim 1\%$ of the previous one. Considering the typical size of other uncertainties in our calculation, we can safely work at LO in this expansion, i.e. at $O(\delta m, \alpha)$.

2.1 Simulation Parameters

We have to fix the four parameters of three flavour QCD, the quark masses m_u, m_d, m_s and the lattice spacing a , setting the bare α to its renormalised value, which is justified in a quenched QED calculation. In order to set the quark masses, we use the observables M_{π^+} to set the average up- and down-quark mass m_{ud} , $M_{K^*}^2 \equiv (M_{K^+}^2 + M_{K^0}^2 - M_{\pi^+}^2)/2$ to set the strange quark mass m_s , $\Delta M_K^2 \equiv M_{K^+}^2 - M_{K^0}^2$ for the isospin breaking of the light quarks δm , and either M_{Ω^-} or the isospin averaged Ξ mass to set the scale. To match valence and sea calculations, we tune m_{ud} and m_s so that M_{π^+} matches the sea pion mass

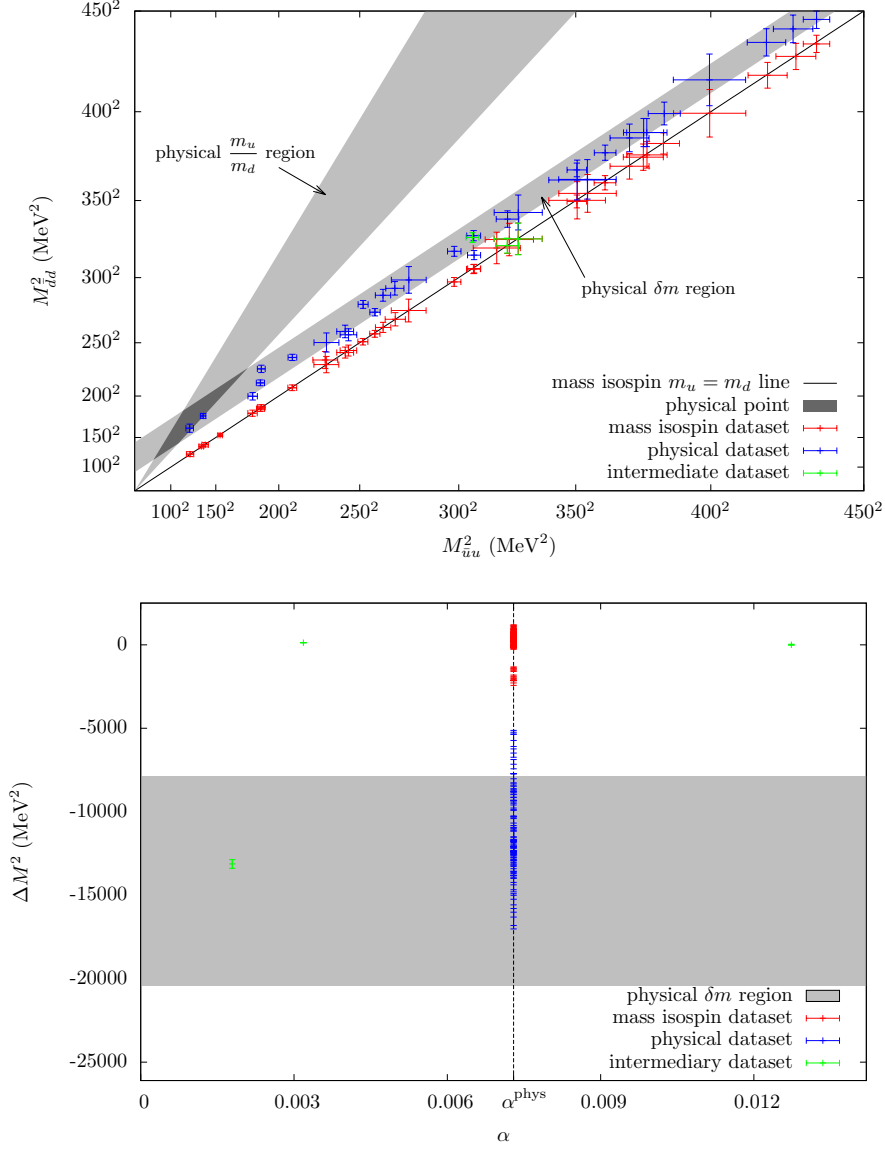


Figure 1. *Top panel:* M_{dd}^2 (see Sec. 2.1) versus M_{uu}^2 landscape plot for the valence datasets produced. For more clarity, the plot was cut above $(450 \text{ MeV})^2$. *Bottom panel:* $\Delta M^2 = M_{uu}^2 - M_{dd}^2$ versus α landscape plot for the datasets produced, α^{phys} marks the physical value.

and M_{K^\times} reproduces it sea value. To that end, we generated three datasets (see Fig. 1). For the first valence dataset we tuned the individual bare up- and down-quark masses such that they are approximatively both equal to the sea light mass. To perform this tuning we had to determine the critical mass shifts in the up- and down-quark mass coming from

the e.m. self-energy¹². In the second valence dataset, m_d is set to be heavier than in the first one simulating the physical splitting δm ; in the third set we vary α in order to be able to separate chiral dependencies with good precision. The lattice spacings are determined simultaneously from a combined fit of the data with $\Delta M \simeq 0$, using techniques described earlier²⁻⁴. The isospin mass splitting ΔM_X of a hadron X is naturally described by the LO isospin expansion:

$$\Delta M_X = A_X \alpha + B_X \Delta M^2, \quad (1)$$

where ΔM^2 substitutes for δm . The coefficients A_X and B_X still depend on the isospin symmetric parameters of the theory, e.g. m_{ud} or m_s . We find that their dependence on these parameters is well described by a linear expansion in $M_{\pi^+}^2$ and in $M_{K^X}^2$ for the range of masses considered here.

The separate e.m. and δm contributions to the baryon mass splittings are interesting in their own right. In order to compute their individual magnitudes, we use the masses of the quark-connected pseudo-scalar mesons $\bar{u}u$ and $\bar{d}d$, with $\delta m = 0$ now implying that their mass difference vanishes: $\Delta M^2 = M_{\bar{u}u}^2 - M_{\bar{d}d}^2 = 0$ (with the remaining parameters tuned to their physical values). Using χ PT results¹³, it is straightforward to show that the difference of these squared masses is $\Delta M^2 = 2B_2\delta m + O(\alpha m_{ud}, \delta m m_{ud}, \alpha \delta m, \alpha^2)$, where B_2 is the $N_f=2$ quark condensate parameter. Close to the physical point, $O(m_{ud})$ can be counted like $O(\delta m)$. This definition of the e.m. contribution, therefore, differs from any other valid one only by higher order terms.

The δm contribution can be obtained by working with $\alpha = 0$, with the other parameters again tuned to their physical values. In particular, the physical value of ΔM^2 is obtained from the analysis of ΔM_K^2 and by computing the value of ΔM^2 corresponding to the physical ΔM_K^2 value^{1,8}.

In Fig. 1 we show the range of parameters used in our study. Our extensive dataset allows us to gain full control on the δm and α dependence of the baryon mass splittings. This is shown in Fig. 2, where we display the ΔM^2 dependence of $\Delta M_\Xi \equiv \Xi^0 - \Xi^-$ and the fully controlled interpolation to the physical value of δm , determined from the experimental measurement of ΔM_K^2 as described above.

We then perform similar interpolations for ΔM_K^2 , $\Delta M_N \equiv M_p - M_n$ and $\Delta M_\Sigma \equiv M_{\Sigma^+} - M_{\Sigma^-}$ as well as all of the other interpolations and extrapolations required to tune to the physical m_{ud} and m_s masses, and to the continuum and infinite volume limits.

2.2 QED

We generate an e.m. field $A_\mu(x)$ for each QCD configuration, using the non-compact e.m. action (in a Coulomb gauge). The action is quadratic and, therefore, the generation of the field straightforward in Fourier space^a. The gauge potential is then fast Fourier transformed back to position space and exponentiated as $U_\mu^{\text{QED}}(x) = \exp(iqeA_\mu(x))$. Unlike the QCD links, our QED links are not smeared before being coupled to quarks. Also, we have not added a clover improvement term for the $U(1)$ field. The $U(1)$ fields are subsequently multiplied with the $SU(3)$ gauge variable on each link and inserted into the Wilson Dirac operator associated with the quark of charge q whose propagator we wish to compute.

^aHere, periodic boundary conditions require subtraction of the zero Fourier mode, $\tilde{A}_\mu(p=0)$ ¹².

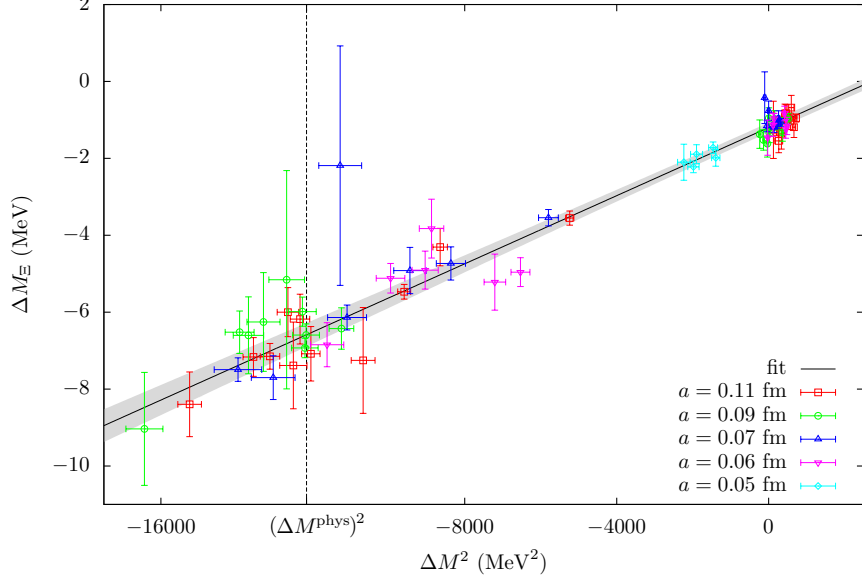


Figure 2. Interpolation of ΔM_{Ξ} to the physical value of δm holding α fixed to its physical value, $(\Delta M^{\text{phys}})^2$ denotes the physical value.

2.3 Finite-Volume Effects

Finite-volume (FV) effects are particularly important in a QED calculation, because of the presence of the massless photon. Using published techniques¹⁴, and performing appropriate asymptotic expansions, it is straightforward to show that the leading finite-volume term in scalar and spinor QED is proportional to $1/L$. These corrections are typically large, as can be expected. In boxes with $L = 1.6 \div 2.6$ fm, which is the largest range of sizes considered in all but one¹⁵ previous studies, the correction to $\Delta_{\text{QED}} M_{\Xi}$, the QED contribution to $\Delta M_{\Xi} \equiv M_{\Xi^0} - M_{\Xi^-}$, ranges from 123 to 76%. This is illustrated in Fig. 3, where we plot our results for $\Delta_{\text{QED}} M_{\Xi}$ as a function of $1/L$. Similar FV corrections are found for QED contributions to other splittings. It is clear that with such corrections one cannot claim to control the extrapolation of QED contributions to infinite volume.

In our calculation L extends up to 6 fm, where we find 36% FV corrections. While still large, these corrections are sufficiently small that they may be described with a low-order polynomial in $1/L$. This is confirmed by the data in Fig. 3, which show no sensitivity to terms beyond linear order in $1/L$. The same features are observed in our results for $\Delta M_N \equiv M_p - M_n$, but with larger statistical errors. Thus we find it sufficient to extrapolate these quantities linearly to the infinite volume limit. The situation is different for $\Delta M_{\Sigma} \equiv \Delta_{[\Delta I_3=2]} M_{\Sigma} = M_{\Sigma^+} - M_{\Sigma^-}$, where the $1/L$ dependence is very small, as expected.

2.4 Discretisation Effects

Concerning discretisation effects, the improvement of the QCD action implies $O(\alpha_s a, a^2)$ corrections to A_X and B_X . However, due to the lack of improvement in the coupling of

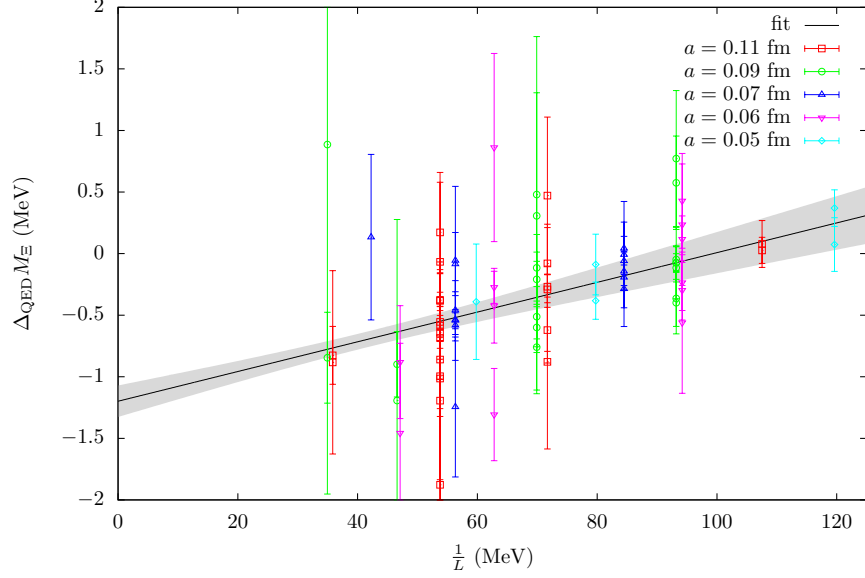


Figure 3. Example of FV corrections to $\Delta_{\text{QED}} M_{\Xi}$, plotted as a function of $1/L$. The dependence of the lattice results on all other variables has been subtracted. Each point type corresponds to one of our five lattice spacings: $a \simeq 0.11$ fm (square), 0.09 fm (circle), 0.07 fm (up triangle), 0.06 fm (down triangle) and 0.05 fm (diamond). The fit, which is linear in $1/L$, is performed with a cut $M_{\pi^+} \leq 500$ MeV. It is plotted as a solid curve, with its 1σ prediction band. It has a $\chi^2/dof = 59./67$.

the photon to quarks, discretisation effects on A_X are $O(a)$. In our analysis, we include $O(a)$ QED discretisation effects to A_X as well as $O(\alpha_s a, a^2)$ QCD ones to B_X .

Combining all of this information yields a 9 parameter description of each of the mass splittings. In the notation of Eq. 1, this corresponds to:

$$A_X = a_0^X + a_1^X [M_\pi^2 - (M_\pi^{\text{phys}})^2] + a_2^X [M_{K^\chi}^2 - (M_{K^\chi}^{\text{phys}})^2] + a_3^X a + a_4^X \frac{1}{L}, \quad (2)$$

$$B_X = b_0^X + b_1^X [M_\pi^2 - (M_\pi^{\text{phys}})^2] + b_2^X [M_{K^\chi}^2 - (M_{K^\chi}^{\text{phys}})^2] + b_3^X f(a) \quad (3)$$

where the a_i^X and b_i^X are the parameters and $f(a) = \alpha_s a$ or a^2 , alternatively. These functional forms characterise the dependence of the mass splittings on the parameters required to reach the physical point and to separate them into δm and e.m. contributions. However, the many competing dependencies make this study particularly challenging.

In our fits we keep only parameters whose fitted values are more than one standard deviation away from zero. For ΔM_K^2 , all parameters are relevant. We also allow for different parameter combinations if they satisfy the previous requirement and not eliminated through their poor fit quality.

2.5 Error Estimation

We follow our histogram based analysis strategy²⁻⁵ to control the systematic uncertainties. Here, we consider the following variations in our analysis procedure. We use two different initial times in our correlator fits, one for which we expect negligible excited state contributions and a second more aggressive one, allowing us to control excited state effects. With the Ω^- and the isospin averaged Ξ we have two ways to set the scale. The uncertainty associated with the truncation of the Taylor expansion used to interpolate these two masses to physical M_{π^+} , is estimated by varying the fit ranges excluding all data with a pion mass above 400 or 450 MeV. To estimate part of the same uncertainty for the isospin splittings, we consider cuts at $M_{\pi^+} = 450$ and 500 MeV, since their $M_{\pi^+}^2$ dependence is very mild. Furthermore, we include either $\alpha_s a$ or a^2 discretisation errors in order to control the systematic uncertainty of our continuum extrapolation. Finally, to estimate any additional uncertainty arising from the truncation of these expansions, we consider the result of replacing either A_X or B_X by Padé expressions. These are obtained by considering that the expansions of A_X and B_X in Eqs. 2-3 are the first two terms of a geometric series which we resume. This resummation is not applied to the FV corrections. Instead we try adding a $1/L^2$ term to either the Taylor or Padé forms. In all cases, we find the coefficient of this term to be consistent with zero.

In total, these different procedures lead to $2^7 = 128$ different fits for each of the isospin splittings and parameter combinations. Correlating these with the 128 fits used to determine $(\Delta M^{\text{phys}})^2$, and allowing various parameter combinations but discarding fits with irrelevant parameters, we obtain between 64 and 256 results for each observable. The central value of a splitting is then the mean of these results, weighted by the p -value; the systematic error is the standard deviation. As usual, the procedure is repeated for 2000 bootstrap samples and the statistical error is the standard deviation of the weighted mean over these samples. The unweighted results differ from the weighted ones by fractions of the respective calculated errors.

Isospin breaking effects not included in the sea are NLO and can, therefore, be safely neglected. The quenching errors related to the neglected $O(\alpha)$ sea-quark contributions are of order $O(1/N_c)$, when large- N_c counting is used. Combining the two suppression factors yields an estimate $(M_\Sigma - M_N)/(N_c M_N) \simeq 0.09$. Smaller estimate can be obtained^{9,16}, however, in the absence of direct quantitative evidence, it is safer to assume that the e.m. contributions to the splittings carry an $O(10\%)$ QED quenching uncertainty.

3 Results and Conclusion

Our main results for the total light hadron octet isospin splittings and their decomposition into QCD (δm) and QED(α) contributions are shown in Tab. 1 and Fig. 4, where we also plot the experimental values. We find good agreement of our results for the total splittings with the ones from experiment.

Through our careful analysis of the different sources of systematic uncertainties, we were able to control all systematic errors with the exception of those due to QED effects on sea quarks. We consider our results to be an encouraging step toward a precise determination of octet baryon splittings, which would constitute an *ab initio* confirmation that the proton cannot decay weakly.

X	ΔM_X	$\Delta_{\text{QED}} M_X$	$\Delta_{\text{QCD}} M_X$
N	$-0.68(39)(36)$	$1.59(30)(35)$	$-2.28(25)(7)$
Σ	$-7.84(87)(72)$	$0.08(12)(34)$	$-7.67(79)(105)$
Ξ	$-7.16(76)(47)$	$-1.29(15)(8)$	$-5.87(76)(43)$

Table 1. Isospin breaking mass differences in MeV for members of the baryon octet. The first error is statistical and the second is systematic. QED quenching uncertainties on the e.m. contributions are estimated to be $O(10\%)$. Propagating the uncertainty in $\Delta_{\text{QED}} M_K^2$ yields an $O(4\%)$ error on the δm contributions. The quenching uncertainties on the total splittings can then be obtained by adding those of the e.m. and δm contributions in quadrature (not included in the results).

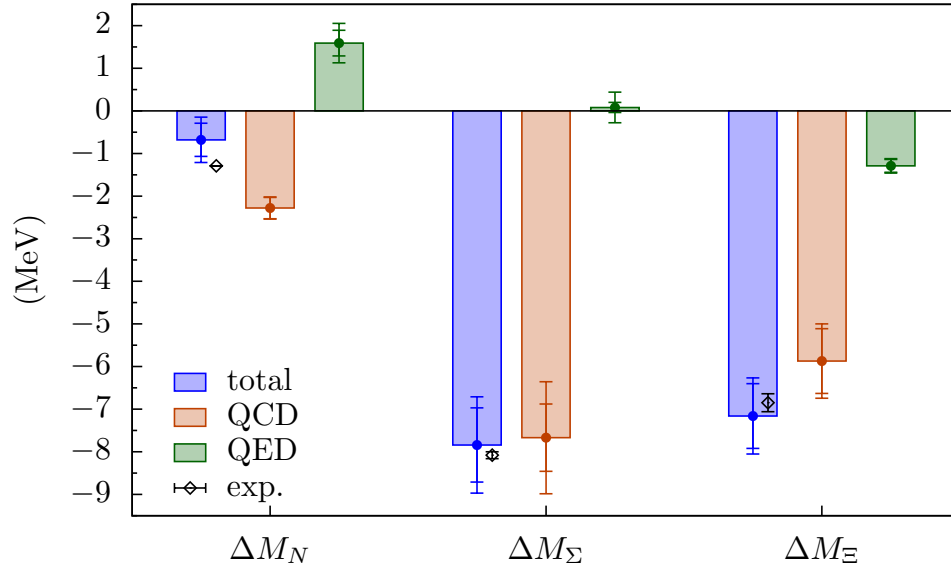


Figure 4. Summary of our results for isospin mass splittings. The total, physical splittings are shown in blue, the QCD (δm) contributions in red and the QED (α) contributions in green. On the points, the error bars are the statistical and total uncertainties (statistical and systematic combine in quadrature). The experimental results are shown as black points.

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